Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[trimethyltin(IV)]-μ-[5-(2-thienylmethyleneamino)-1,3,4-thiadiazole-2-thiolato-κ^2N^4:S^2]]

Junshan Sun, Rufen Zhang* and Daqi Wang

Department of Chemistry, Liaocheng University, Liaocheng 252059, People's Republic of China

Correspondence e-mail: macl@lcu.edu.cn

Received 31 December 2006
Accepted 2 January 2007

The Sn atom in the linear polymeric chain structure of the title complex, $[Sn(CH_3)_3(C_7H_4N_3S_3)]_n$, is in a *trans*-$C_3SnNS$-trigonal bipyramidal geometry.

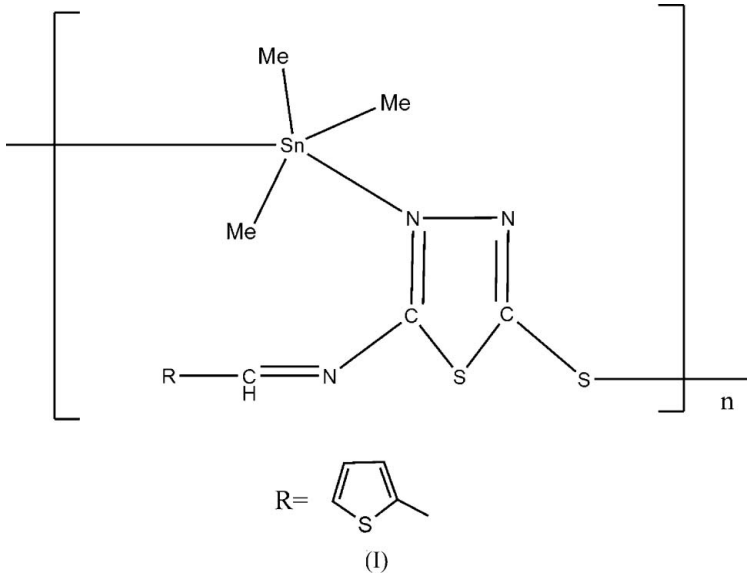
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.035
wR factor = 0.122
Data-to-parameter ratio = 17.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Schiff bases derived from heterocycles possess antibacterial and anticancer activity (Kiran, *et al.*, 2006). There have been numerous studies on metal complexes of *S*,*N* chelating agents such as those derived from the *S*-alkyl/aryl esters of dithiocarbazic acid and thiosemicarbazones (West, *et al.*, 1991). Most studies involve complexes with transition metals. Complexes of main group metals have been studied less. In recent years, organotin(IV) complexes of Schiff bases ligands containing *S*,*N* donor atoms have received much attention because of the ability of tin to bind with S or N atoms. We selected a ligand containing the triazole unit and report here a new triorganotin(IV) complex, (I).



(I)

In complex (I), the Sn atom has a trigonal bipyramidal coordination (Fig. 1); three methyl groups define the equatorial plane. The N2^{i}—Sn1—S2 angle is 172.38 (12)°, slightly distorted from the normal axis of 180°. The Sn1—S2 bond is longer than the covalent radii of Sn and S (2.42 Å; James, *et al.*, 1994), but much shorter than the sum of the van der Waals radii of Sn and S (4.0 Å; Casas, *et al.*, 1997). In addition, the Sn1—N2 distance lies in the normal range (Zhang *et al.*, 2005). The compound adopts a linear chain motif that runs along the *b*-axis direction.

© 2007 International Union of Crystallography
All rights reserved

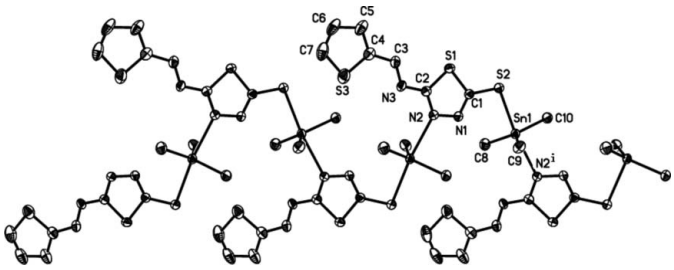


Figure 1
The polymeric structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted. [Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.]

Experimental

Trimethyltin chloride, 5-amino-1,3,4-thiadiazole-2-thiol and 2-thiophenecarboxaldehyde were commercially available. The Schiff base ligand was synthesized according to a reported procedure (Burns *et al.*, 1968). The reaction was carried out under a nitrogen atmosphere. The Schiff base ligand (0.227 g, 1 mmol) was added to a solution of sodium ethoxide (0.272 g, 1 mmol) in 30 ml benzene, and the mixture was stirred for 10 min; trimethyltin chloride (0.199 g, 1 mmol) was then added. Caution! trimethyltin chloride is toxic. The reaction mixture was kept at 313 K for 12 h. After cooling to room temperature, the solution was filtered. The solvent was removed from the filtrate under vacuum, and the solid residue was recrystallized from diethyl ether; yellow crystals suitable for X-ray diffraction studies were obtained (yield 0.550 g, 80%; m.p. 452 K). Analysis, calculated for $C_{10}H_{13}N_3S_3Sn$: C 30.79, H 3.36, N 10.77; found: C 30.62, H 3.58, N 10.54%. The elemental analyses were performed with a PE2400II apparatus.

Crystal data

$[Sn(CH_3)_3(C_7H_4N_3S_3)]$	$Z = 8$
$M_r = 390.10$	$D_x = 1.742$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 13.068$ (6) Å	$\mu = 2.12$ mm^{-1}
$b = 11.294$ (5) Å	$T = 298$ (2) K
$c = 20.158$ (9) Å	Block, yellow
$V = 2975$ (2) Å^3	0.32 × 0.23 × 0.14 mm

Data collection

Bruker SMART area-detector diffractometer	14610 measured reflections
φ and ω scans	2626 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1760 reflections with $I > 2\sigma(I)$
$T_{min} = 0.550$, $T_{max} = 0.756$	$R_{int} = 0.041$
	$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 9.0072P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.035$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.122$	$\Delta\rho_{max} = 0.74$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.62$ e Å^{-3}
2626 reflections	
154 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—C9	2.117 (7)	Sn1—N2^{i}	2.579 (5)
Sn1—C8	2.125 (7)	Sn1—S2	2.614 (2)
Sn1—C10	2.128 (6)	N2—Sn1^{ii}	2.579 (5)
C9—Sn1—C8	122.7 (3)	C10—Sn1—N2^{i}	84.8 (2)
C9—Sn1—C10	119.3 (3)	C9—Sn1—S2	96.0 (2)
C8—Sn1—C10	116.0 (3)	C8—Sn1—S2	97.5 (2)
C9—Sn1—N2^{i}	81.7 (2)	C10—Sn1—S2	90.04 (19)
C8—Sn1—N2^{i}	89.8 (2)	N2^{i}—Sn1—S2	172.38 (12)

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

H atoms were positioned geometrically, C–H 0.93–0.96 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (20271025) for financial support.

References

Burns, G. R. (1968). *Inorg. Chem.* **7**, 277–283.
Casas, J. S., Castineiras, A., Martinez, E. G., Gonzalez, A. S. & Sanchez, A. (1997). *Polyhedron*, **16**, 795–800.
James, B. D., Magee, R. J., Patalinghug, W. C., Skelton, B. W. & White, A. H. (1994). *J. Organomet. Chem.* **467**, 51–54.
Kiran, S., Manjeet, S. B. & Parikshit, T. (2006). *Eur. J. Med. Chem.* **41**, 147–153.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
West, D. X., Padhye, S. B. & Sonawane, P. B. (1991). *Struct. Bond.* **76**, 1–4.
Zhang, R. F., Tian, G. R. & Ma, C. L. (2005). *J. Organomet. Chem.* **690**, 4049–4057.